Polarization Analysis Based on Realistic Lithium Ion Battery Electrode Microstructure Using Numerical Simulation

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The performance of lithium ion battery (LIB) is limited by the inner polarization and it is important to understand the factors that affect the polarization. This study focuses on the polarization analysis based on realistic 3D electrode microstructures. A c++ software was developed to rebuild and mesh the microstructure of cathode and anode electrodes through Nano-CT and Micro-CT scanned images respectively. As a result, the LIB model was composed of electrolyte, cathode and anode active materials and current collectors. By employing 3D finite volume method (FVM), another c++ code was developed to simulate the discharge and charge processes by solving coupled model equations. The simulation revealed the distribution of physical and electrochemical variables such as concentration, voltage, current density, reaction rate, et al. In order to explore the correlation of local effects and electrode structural heterogeneity, the cathode electrode were divided equally into 8 sub-divisions, of which the porosity, tortuosity, specific surface area were calculated. We computed the polarizations in the sub-divisions due to different sub-processes, i.e., the activation of electrochemical reactions and charge transport of species. As shown in Fig. 1, the tortuosity is very irregular because of unevenly distributed cathode particle size and packing pattern with low porosity. There are no exact and direct relations among porosity, tortuosity and specific surface area. Fig. 2 shows that the polarizations are related to the porosity in sub-divisions. The knowledge from the study will help to figure out the mechanism of polarization and power loss in LIB, which could be useful to improve LIB design and manufacturing. Acknowledgments: This work was supported by US National Science Foundation under Grant No. 1335850.

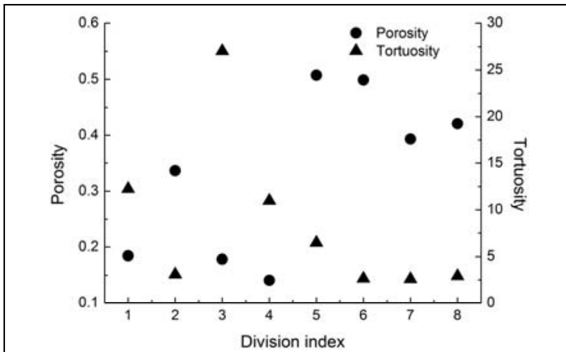

Fig. 1 Porosity and tortuosity in sub-divisions of a cathode electrode

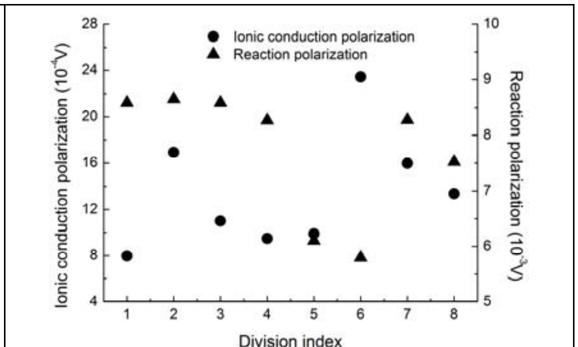

Fig. 2 Intercalation reaction polarization and ionic conduction polarization of sub-divisions at 120 sec during a 5 C charging process

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